FELIX: The Albany Ice Sheet Modeling Code

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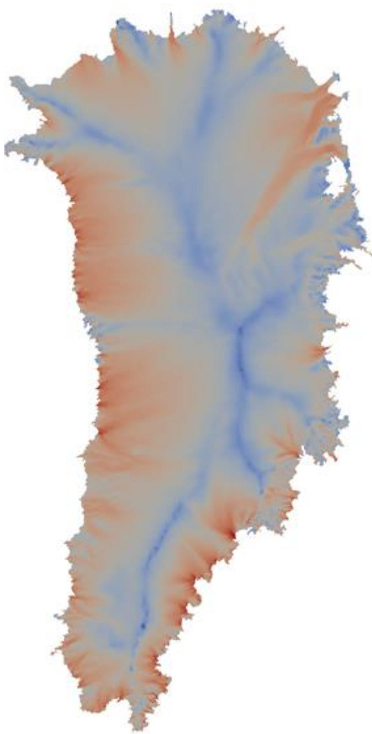

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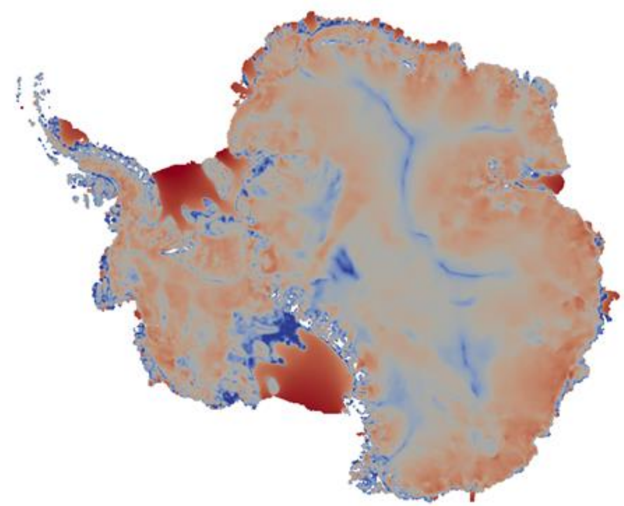
Albany User Group Meeting
January 15-16, 2014

Sandia National Laboratories
Albuquerque, NM



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The PISCEES Project

FSU FELIX
FSU
Finite Element
Full Stokes Model

PISCEES
SciDaC Application Partnership
(DOE's BER + ASCR divisions)
Start date: June 2012

3 land-ice dycores developed under PISCEES

Albany/FELIX
SNL
Finite Element
"Higher-Order" Stokes Model

Increased fidelity

BISICLES
LBNL
Finite Volume
L1L2 Model

Goal: support DOE climate missions (sea-level rise predictions)

PISCEES: Predicting Ice Sheet Climate & Evolution at Extreme Scales
FELIX: Finite Elements for Land Ice eXperiments
BISICLES: Berkeley Ice Sheet Initiative for Climate at Extreme Scales

Albany/FELIX & Agile Components Code Development Strategy

Albany/FELIX is a(nother) success story for the **Agile Components** code development strategy and the **Albany** code base!

Agile Components/Albany have enabled ***rapid development*** of new application code!

In ***1.5 calendar years/1.5 FTEs of effort***, we:

- Wrote the FELIX "higher-order" Stokes dycore.
- Verified this new code.
- Got real data into new code for science runs.
- Performed analysis of and with the new code.

Talk Outline

The Ice Sheet PDEs: "Higher-Order Stokes" Model

- New physics added to Albany:
  - "***Higher-order" Stokes PDEs***: two coupled nonlinear PDEs for u and v velocities of the ice with Glen's law viscosity μ.

$$\begin{cases} -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_1) = -\rho g \dfrac{\partial s}{\partial x} \\ -\nabla \cdot (2\mu \dot{\boldsymbol{\epsilon}}_2) = -\rho g \dfrac{\partial s}{\partial y} \end{cases}, \quad \text{in } \Omega$$

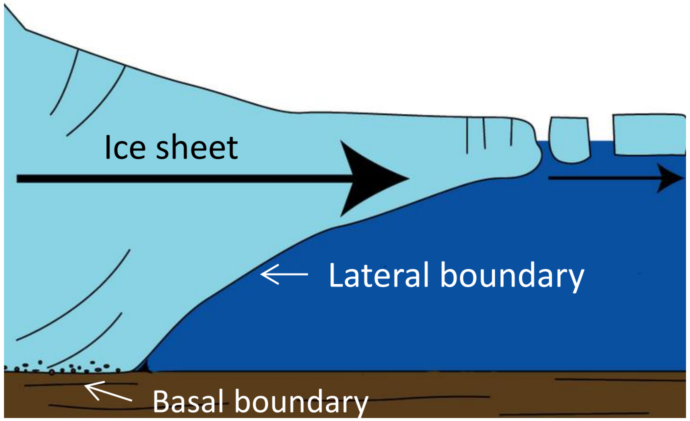
$$\dot{\boldsymbol{\epsilon}}_1{}^T = (2\dot{\epsilon}_{11} + \dot{\epsilon}_{22}, \dot{\epsilon}_{12}, \dot{\epsilon}_{13})$$
$$\dot{\boldsymbol{\epsilon}}_2{}^T = (2\dot{\epsilon}_{12}, \dot{\epsilon}_{11} + 2\dot{\epsilon}_{22}, \dot{\epsilon}_{23})$$
$$\dot{\epsilon}_{\mathrm{ij}} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial uj}{\partial xi}\right)$$

- New boundary conditions added to Albany:
  - ***Basal sliding BC:*** $2\mu \dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} + \beta u_i = 0$, on Γ_β

$$\boxed{\beta = \text{sliding coefficient} \geq 0}$$

  - ***Floating ice BC:***

$$2\mu \dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} = \begin{cases} \rho g z \boldsymbol{n}, & \text{if } z > 0 \\ 0, & \text{if } z \leq 0 \end{cases}$$



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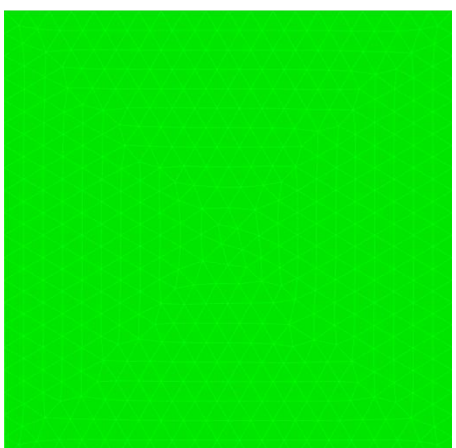
Verification #1: Convergence Study on MMS Problems

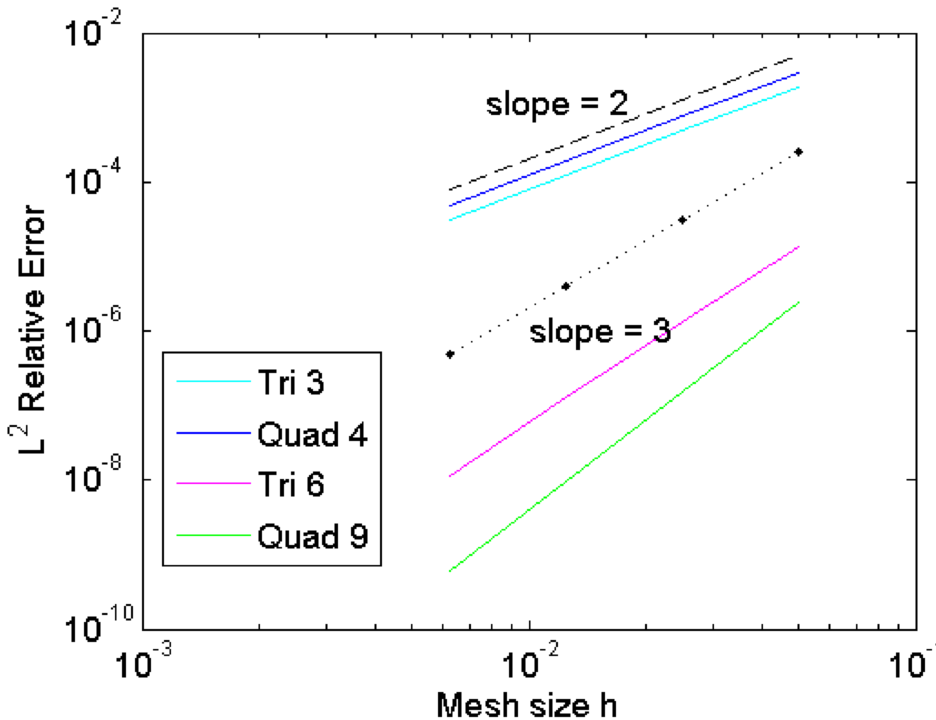
- ***2D Method of Manufactured Solutions (MMS) problem***: source terms f_1 and f_2 are derived such that

$$u = \sin(2\pi x)\cos(2\pi y) + 3\pi x$$
$$v = -\cos(2\pi x)\sin(2\pi y) - 3\pi y$$

is the exact solution to

$$-\nabla \cdot (2\mu\dot{\boldsymbol{\epsilon}}_1) = f_1$$
$$-\nabla \cdot (2\mu\dot{\boldsymbol{\epsilon}}_2) = f_2$$

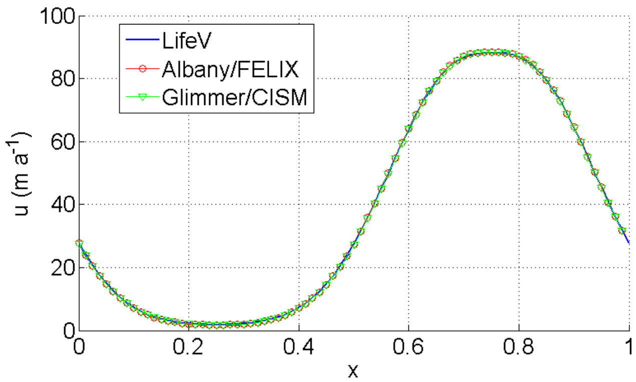




- All elements tested attain expected convergence rates (above).
- Unstructured meshes not a problem for the FEM! (left)

Verification #2: Code-to-Code Comparisons on Canonical Benchmarks

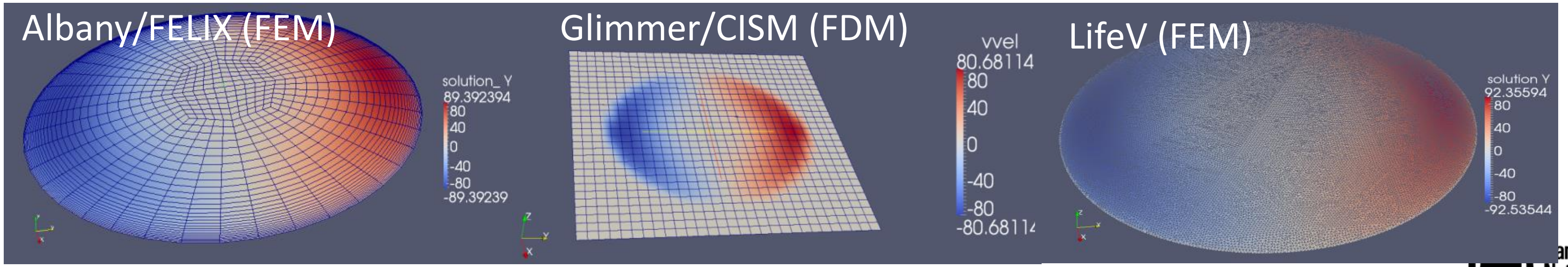
- ***ISMIP-HOM Test A:*** Test case on transformed box domain.



***Collaborators**:*
A. Salinger, M. Perego (SNL);
S. Price, W. Liscomb (LANL)

Agreement between Albany/FELIX and other solutions is excellent!

- ***Dome Test Case:*** Test case that simulates 3D flow field within an isothermal, parabolic shaped dome of ice with circular base.



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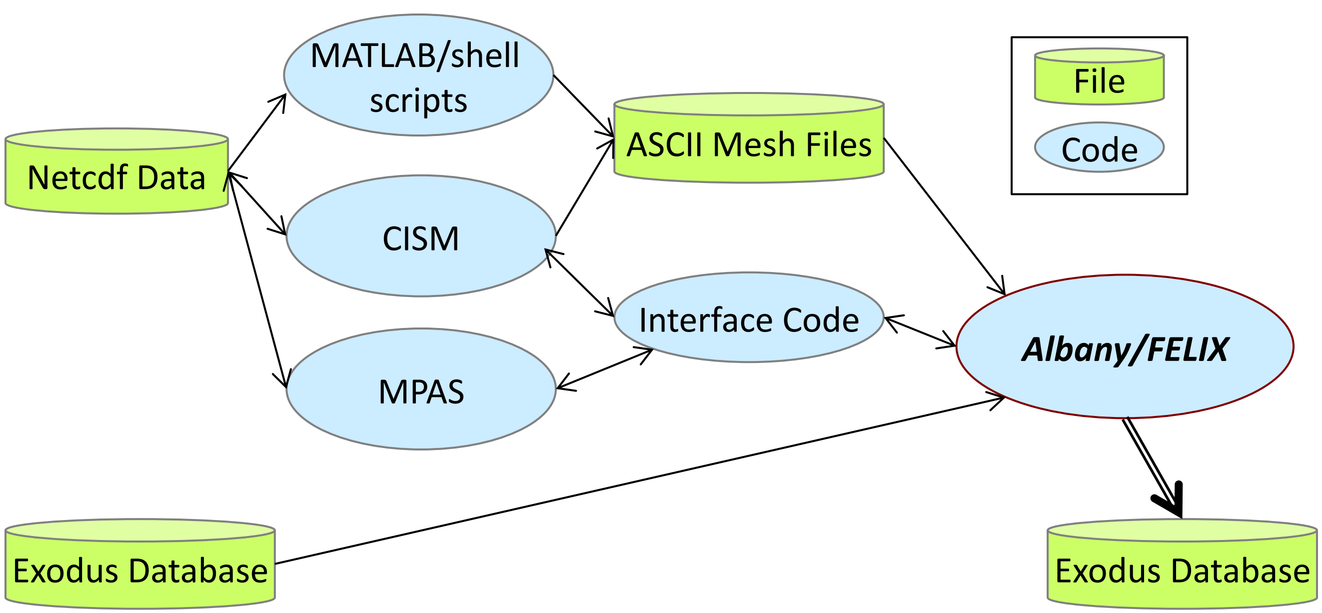
Importing Real Data into Albany/FELIX

Data (geometry, topography, surface height, basal traction, temperature, etc.) needs to be imported into Albany to run "real" problems (Greenland, Antarctica).

- ***Approach 1 to get data into Albany***: Exodus file → Albany.
- ***Approach 2 to get data into Albany:*** Netcdf file → ASCII file → Albany STK ASCII Mesh Reader → Albany.

```
<ParameterList name="Discretization">
  <Parameter name="Method" type="string" value="Ascii"/>
  <Parameter name="Exodus Output File Name" type="string" value="gis20km_ascii_out.exo"/>
</ParameterList>
```

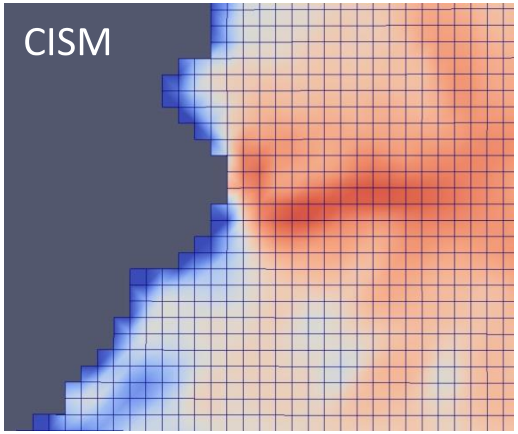
- ***Approach 3 to get data into Albany:*** Netcdf file → run CISM/MPAS → Albany interface → Albany.

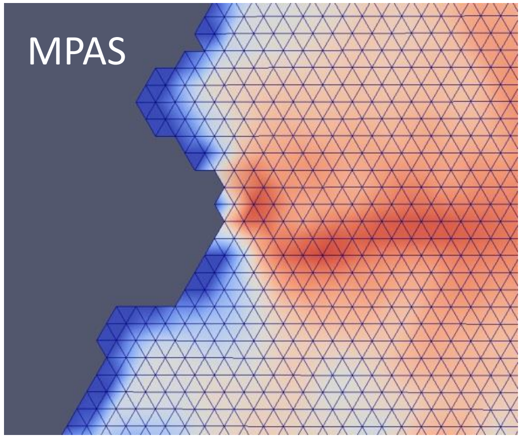


Additions to Albany:

- Parallel ASCII mesh readers (M. Perego, I. Kalashnikova).
- Interfaces to MPAS (M. Perego) & CISM (I. Kalashnikova).

Importing Real Data into Albany/FELIX (cont'd): Meshes





We have run Albany/FELIX with several kinds of meshes

- **Structured hexahedral** meshes (compatible with CISM) – *top left*
- **Structured tetrahedral** meshes (compatible with MPAS) – *bottom left*
- True **unstructured Delaunay triangle** meshes – *right*

Albany/FELIX + interfaces is up and running on ***Hopper*** (NERSC) and ***Titan*** (ORNL)!

Unstructured Delauney Triangle

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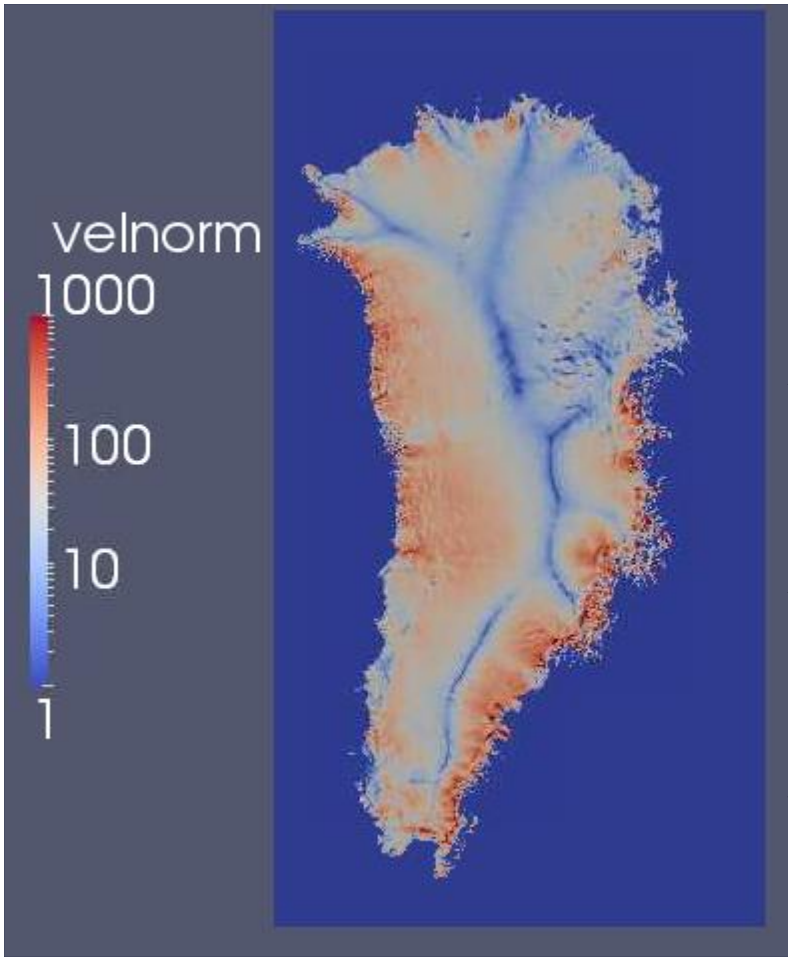
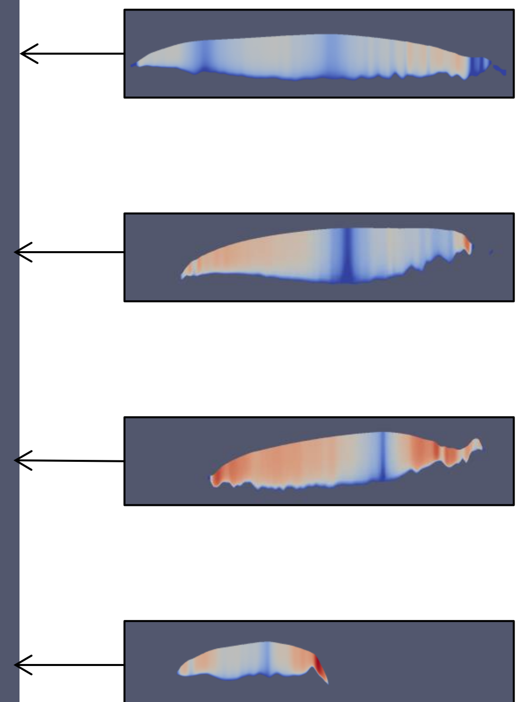
Structured Hexahedral Grid Results (CISM-Albany Interface)



Surface velocity magnitude [m/yr]



Velocity magnitude [m/yr] in x-z planes. (height "z" is stretched 100x.)

1 km resolution "new" (9/25/13) Greenland dataset

16.6M hex elements
37M unknowns

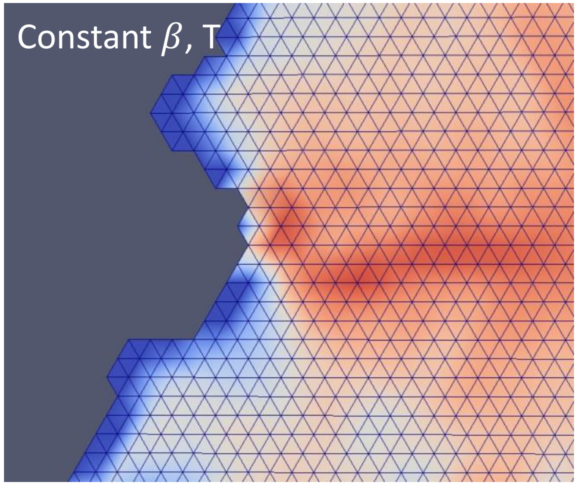
constant β, T
(no-slip)

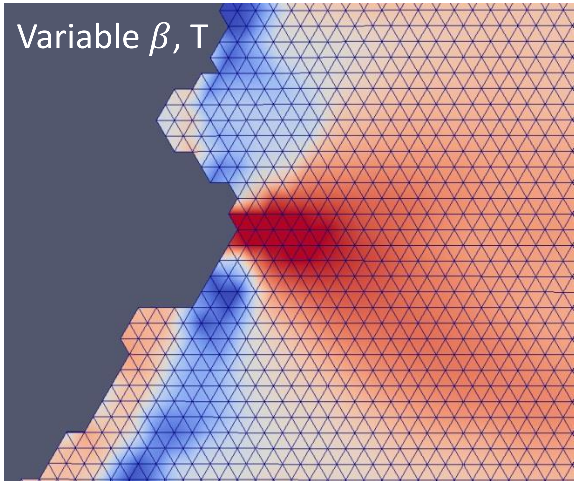
Data set courtesy of M. Norman (ORNL)

Albany/FELIX was ***first*** code to converge on this (fine) resolution problem!

Structured Tetrahedral Grid Results (MPAS-Albany Interface)

Greenland (Jakovshavn close-up)

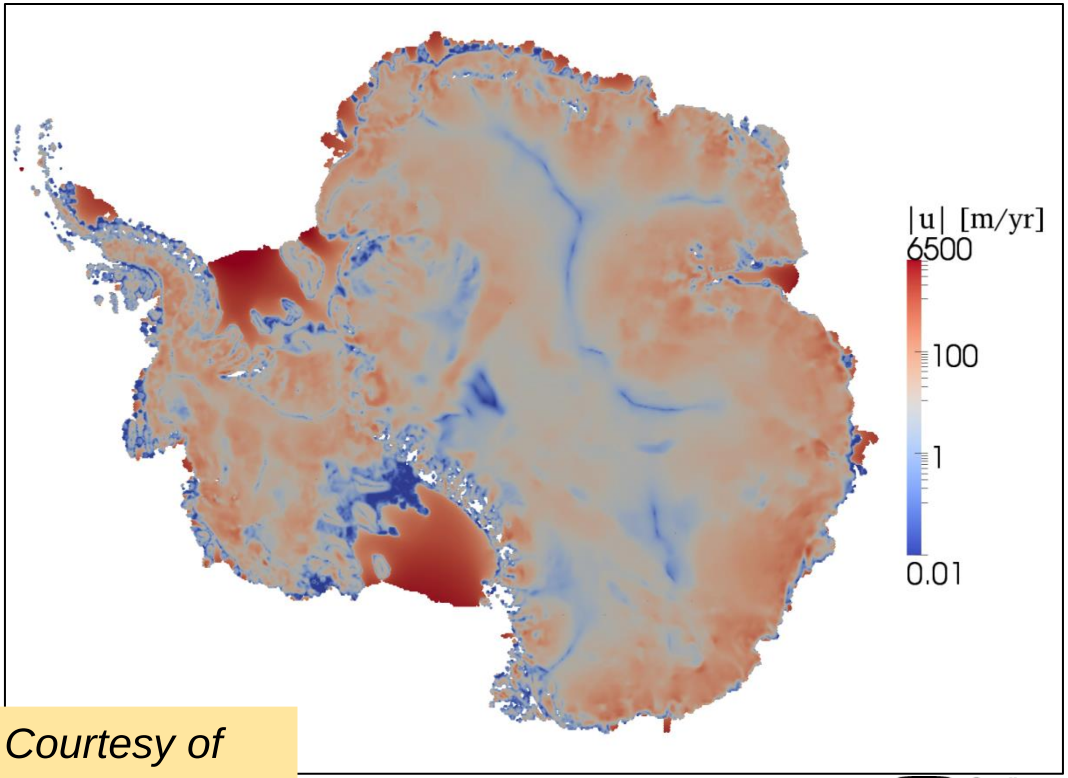




Antarctica (10 km)

$$\beta = \begin{cases} 10^5 \text{ [Land]} \\ 10^{-5} \text{ [Floating]} \end{cases}$$

Temperature = Linear



Courtesy of M. Perego (SNL)

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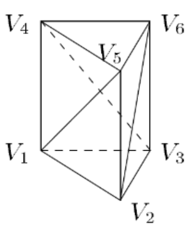
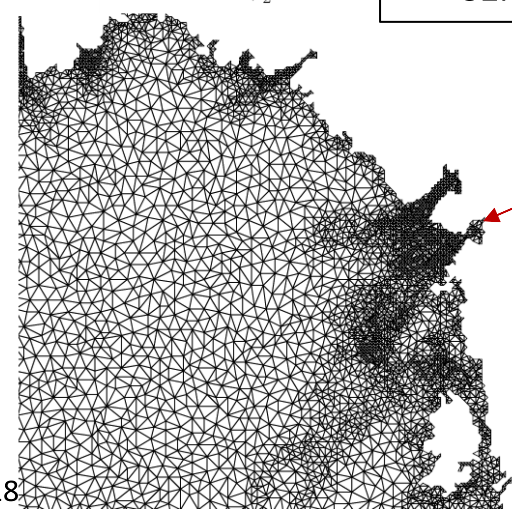
Unstructured Delaunay Triangle Grid Results

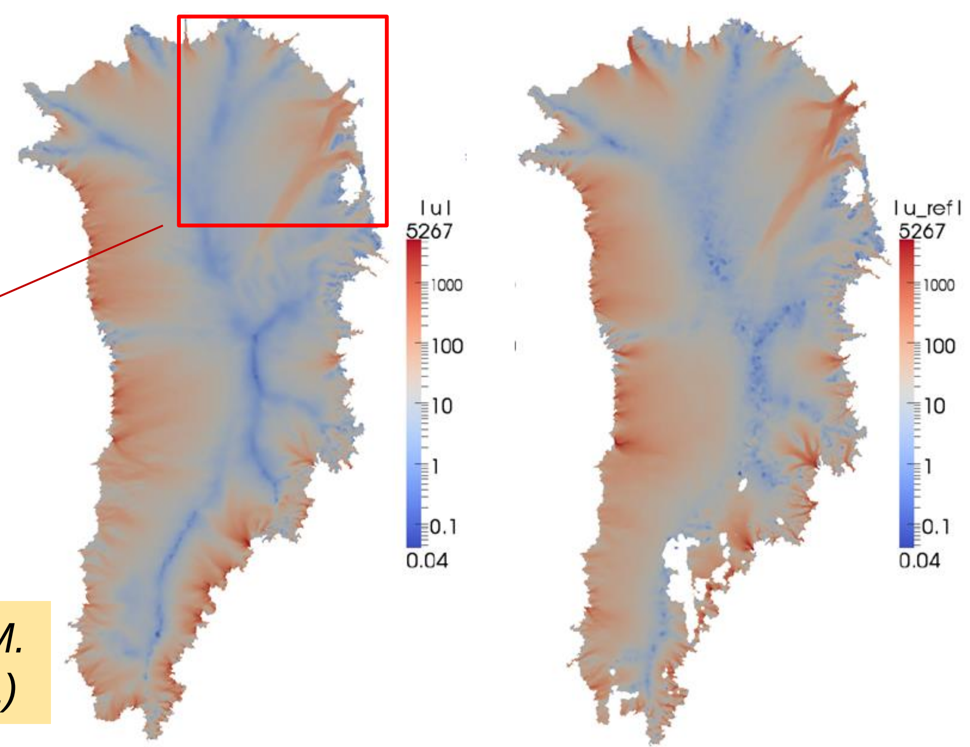
- **Step 1:** determine geometry boundaries and possible holes ***(MATLAB)***.
- **Step 2:** generate uniform triangular mesh and refine based on ***gradient of measured surface velocity (Triangle – a 2D meshing software).***
- **Step 3:** obtain 3D mesh by extruding the 2D mesh in the vertical direction as ***prism***, then splitting each prism into 3 ***tetrahedra (Albany).***



Mesh Details
Min h: 4 km
Max h: 15 km
32K nodes

|computed surface velocity| [m/yr] |reference surface velocity| [m/yr]





Courtesy of M. Perego (SNL)

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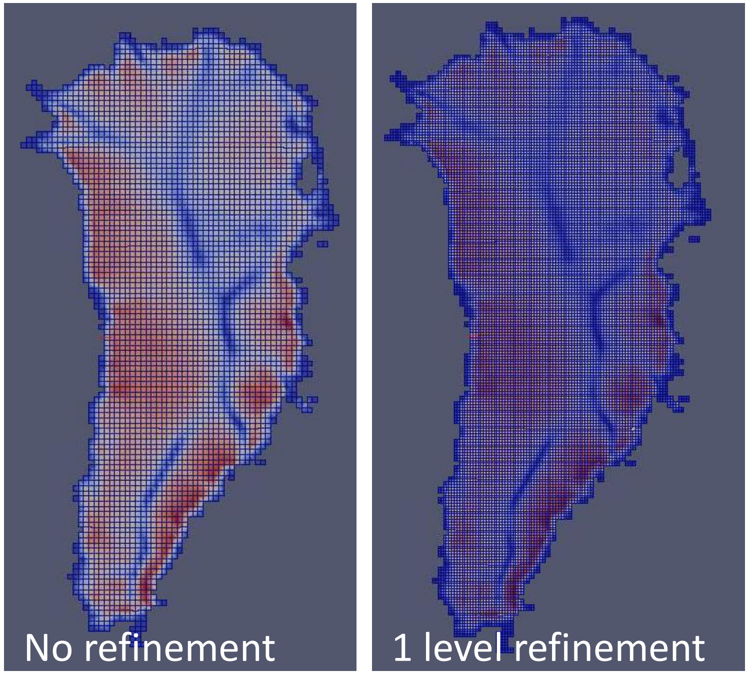
Verification #3 (on-going effort): Convergence Study using Albany Adaptivity

Why?

- Verify order of convergence *$O(h^2)$*.
- Get an idea of the discretization error.
- Study refinement in vertical levels.
- Perform controlled scalability study.

How?

- Fix geometry and data from Greenland.
- Bisect mesh in 3D using uniform mesh-refinement capability in Albany's Adaptivity class.
- Repeat.



Preliminary Result: 20 km Greenland

# Levels Refinement	|solution average|
none	2.682274
1 level	3.0067294
2 levels	3.145237

With help from G. Hansen (SNL)

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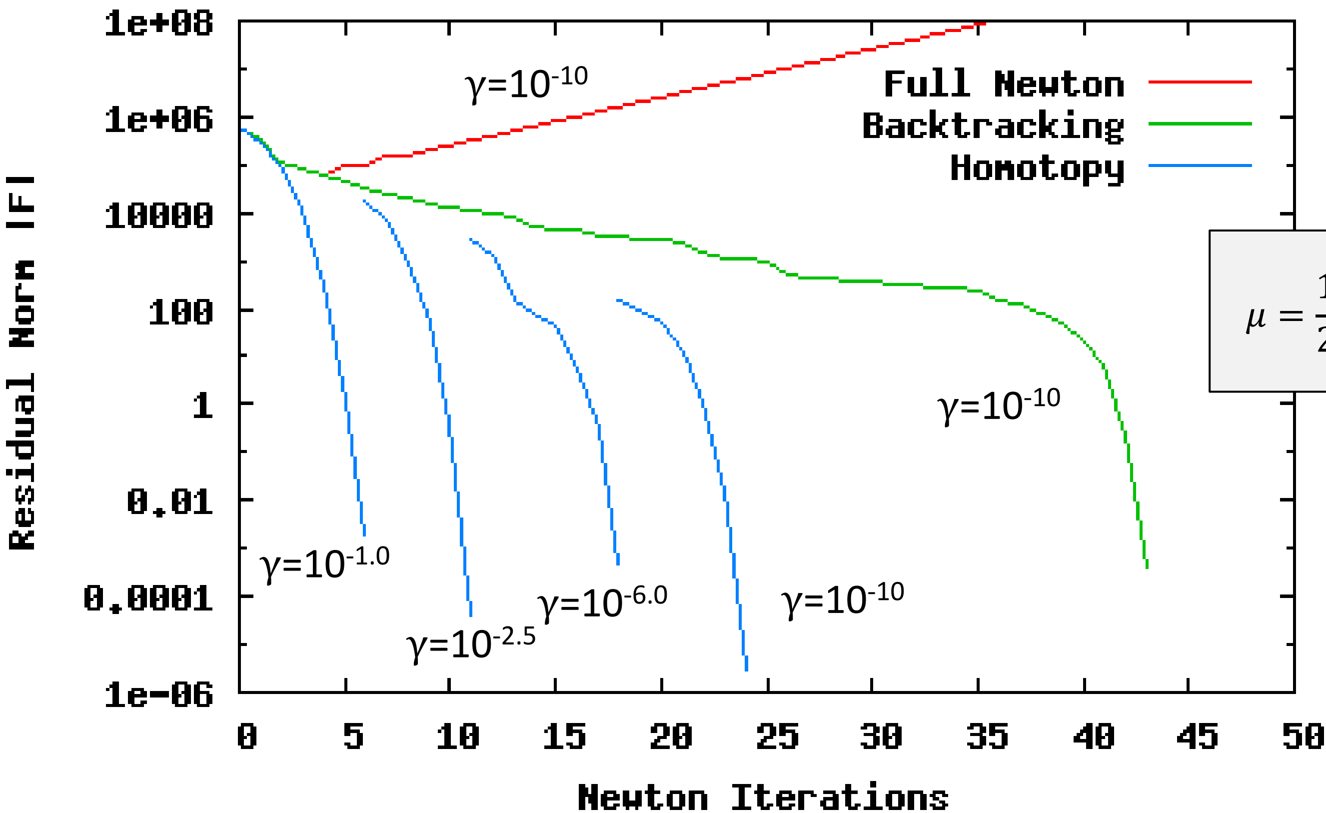
Robustness of Newton's Method via Homotopy Continuation (LOCA)



Glen's Law Viscosity:

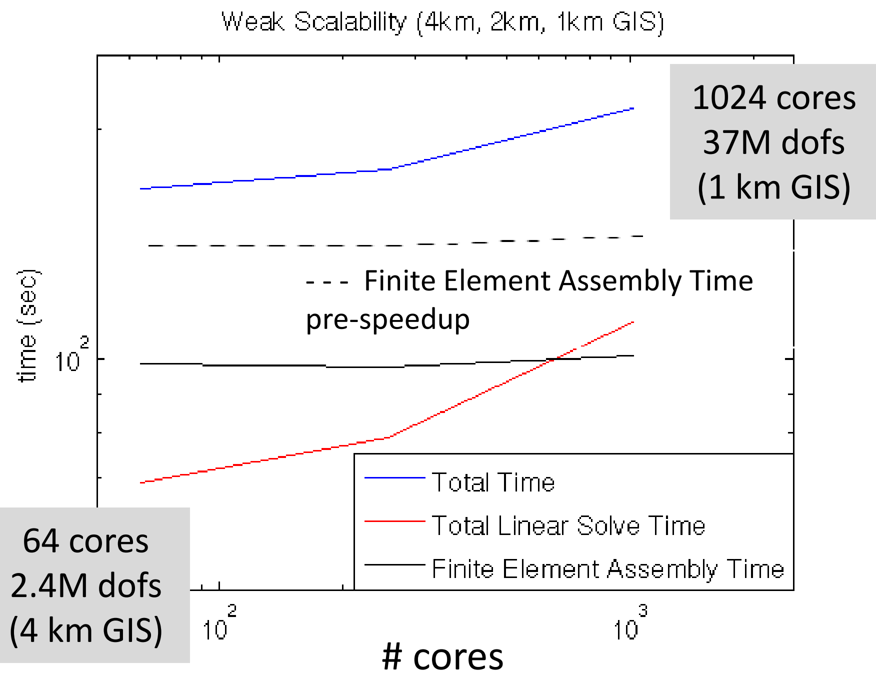
$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2} \sum_{ij} \dot{\epsilon}_{ij}^{\,2} + \gamma \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

$\gamma =$ regularization parameter

- Newton's method most robust with full step + homotopy continuation of $\gamma \rightarrow 10^{-10}$: converges out-of-the-box!

Weak and Strong Scalability (on Hopper)

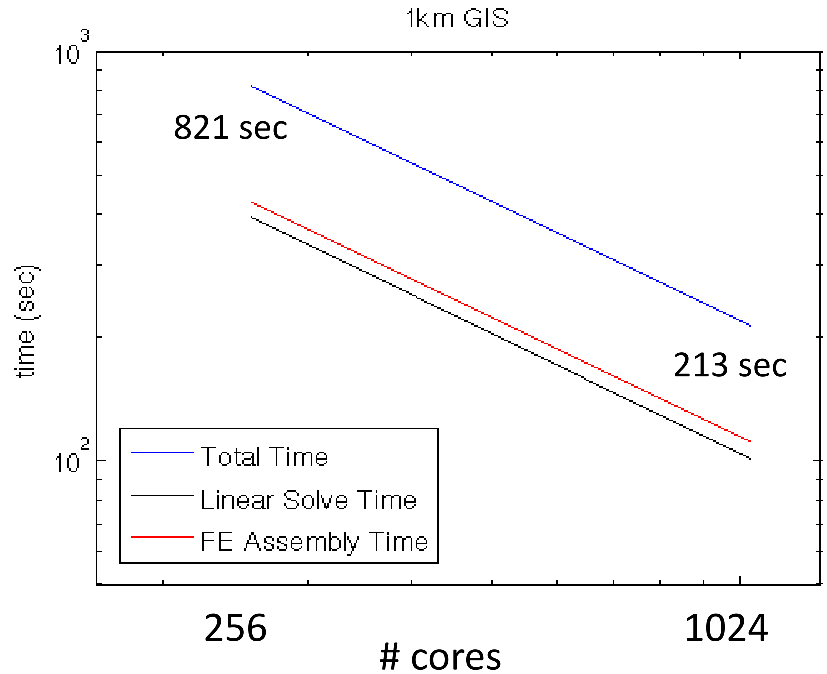
Weak Scalability



- Figure above shows weak scaling (with changing data, ~37K dofs/core) for 9/25/13 4 km→1 km Greenland data sets with no-slip at bedrock.

Courtesy of R. Tuminaro (SNL)

Strong Scalability



- Strong scaling study above for 1 km with no-slip at bedrock (37M Unknowns): 3.86x speedup with 4x cores.
- Only 213 sec on 1024 cores, including homotopy.

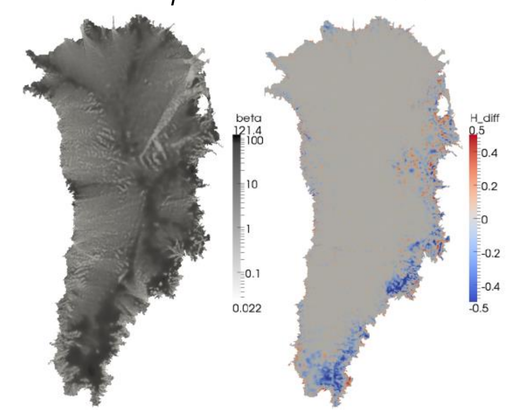
Deterministic Inversion: Estimation of Ice Sheet Initial State

Higher-Order Stokes PDE Constrained Optimization Problem:

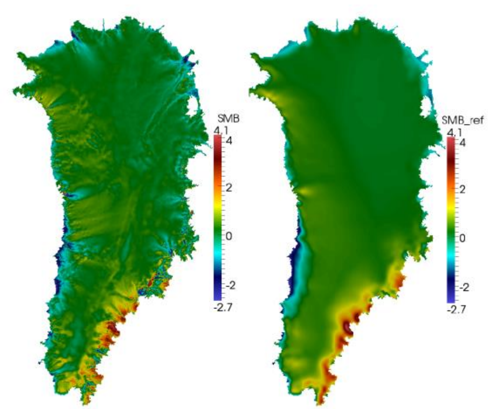
$$J(\beta, H) = \frac{1}{2}\alpha \int_{\Gamma} |div(\boldsymbol{U}H) - SMB|^2 ds + \frac{1}{2}\alpha_v \int_{\Gamma top} |\boldsymbol{u} - \boldsymbol{u}^{obs}|^2 ds + \frac{1}{2}\alpha_H \int_{\Gamma top} |H - H^{obs}|^2 ds + \mathcal{R}(\beta) + \mathcal{R}(H)$$

- Minimize difference between:
  - Computed divergence flux and measured ***surface mass balance (SMB)***.
  - Computed and measured ***surface velocity ($\boldsymbol{u}^{obs}$)***.
  - Computed and ***reference thickness (H^{obs})***.
- Control variables:
  - ***Basal friction (β)***.
  - ***Thickness (H)***.
- Software tools: ***LifeV*** (assembly), ***Trilinos*** (linear/nonlinear solvers), ***ROL*** (gradient-based optimization).

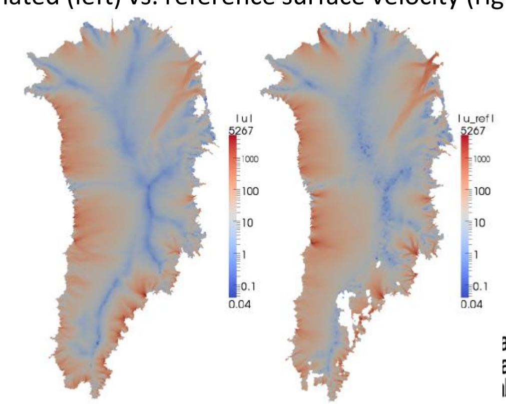
Estimated β $H - Hobs$



Estimated divergence (left) vs. reference SMB (right)



Estimated (left) vs. reference surface velocity (right)



Courtesy of: *M. Perego (SNL); S. Price (LANL); G. Stadler (UT)*

Bayesian Inversion: Moderate-Dimensional Greenland Problem

- Albany/FELIX has been hooked up to ***DAKOTA/QUESO*** (in "black-box" mode) for ***UQ/Bayesian inference.***

Difficulty in UQ: "Curse of Dimensionality"
The β-field inversion problem has $O(20{,}000)$ dimensions!

- Reduce $O(20{,}000)$ dimensional problem to $O(5)$ dimensional problem using ***Karhunen-Loeve Expansion (KLE)***:

Offline

1. Assume analytic covariance kernel $C(r_1, r_2) = exp\left(-\frac{(r_1 - r_2)^2}{L^2}\right)$.
2. Perform eigenvalue decomposition of C.

Online

3. Expand β in basis of eigenvectors $\{\boldsymbol{\phi}_k\}$ of C, with random variables $\{\xi_k\}$:

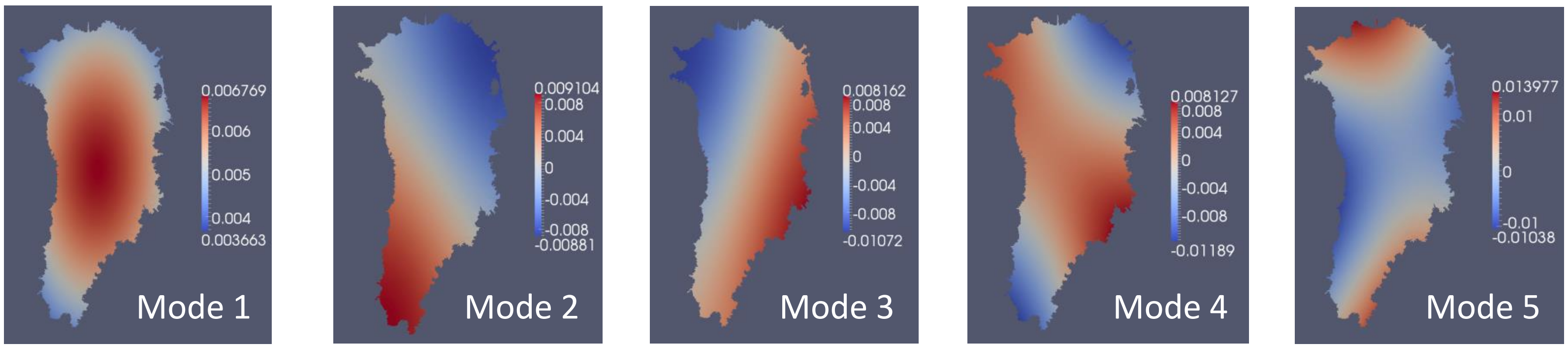
$$\boxed{log(\beta(\omega)) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{\lambda_k}\boldsymbol{\phi}_k \xi_k(\omega)}$$

Collaborators:
A. Salinger,
L. Swiler,
M. Eldred,
J. Jakeman (SNL)

Inference/calibration is for coefficients of KLE
$\Rightarrow$ ***significant dimension reduction***.

Preliminary Results for Greenland Bayesian Inference

- 5 KLE modes capture 95% of covariance energy → parallel C++/Trilinos code (**Anasazi**).



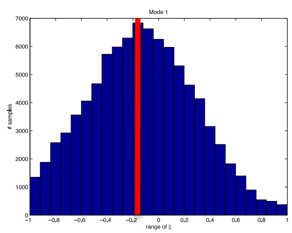
- Mismatch = sum of squares of surface velocity discrepancy → **Albany.**
- Polynomial chaos expansion (PCE) was formed for the mismatch over ξ_k using uniform prior distributions and isotropic sparse grid level = 3 → **DAKOTA**.
- Markov Chain Monte Carlo (MCMC) was performed on the PCE with 100K samples → **QUESO**.

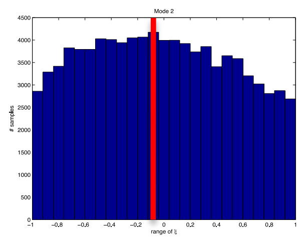
***Collaborators**: M. Perego, J. Jakeman, M. Eldred, L. Swiler (SNL)*

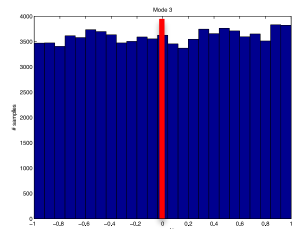
Preliminary Results for Greenland Bayesian Inference (cont'd)

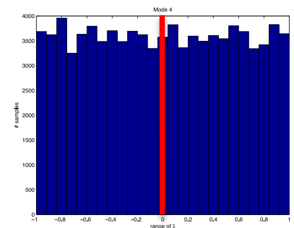
MAP solution:
$x = (-0.16, -0.08, 0, 0, 0)$

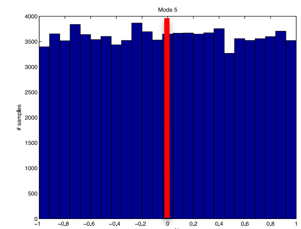
- Posterior distributions for the 5 KLE coefficients:


Coefficient 1

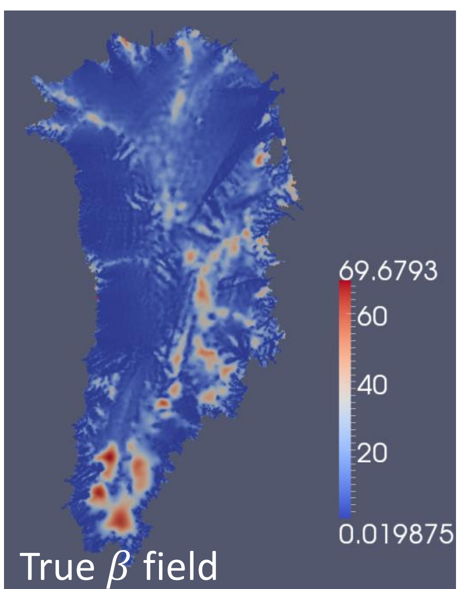

Coefficient 2


Coefficient 3


Coefficient 4


Coefficient 5

- Inference of KLE random field:

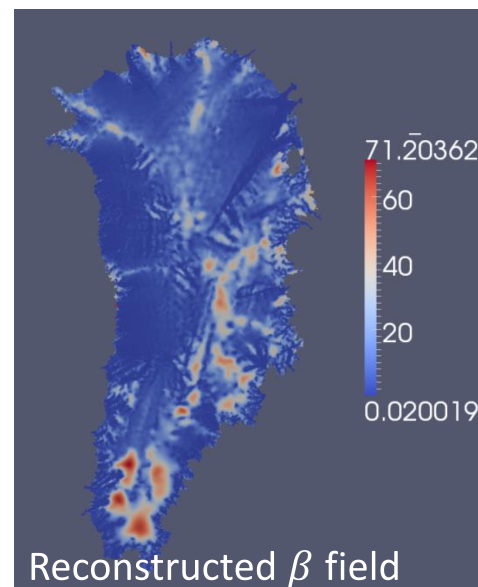


True β field

Left: true β field

Right: *reconstructed β field*

Good agreement between true and reconstructed β field!



Reconstructed β field

Summary and Future Work

Summary:

- Development of new finite element land ice dycore ("FELIX") is underway within Albany.
- "Higher-order" Stokes PDE, and various boundary conditions (sliding BC, floating BC) have been implemented in Albany.
- Albany framework and Agile Components code development strategy has enabled rapid development of this code!

Verification, science simulations, scalability, robustness, UQ, advanced analysis: all attained in **~1.5 FTE of effort**!

Ongoing/future work:

- Dynamic simulations of ice evolution.
- Adjoint-based sensitivities.
- Conversion to new Kokkos array for hybrid/new architecture machines.
- Delivering code to users in climate community.
- Coupling to community earth system model (CESM).

Thank you! Questions?

References

[1] M.A. Heroux *et al.* "An overview of the Trilinos project." *ACM Trans. Math. Softw.* **31**(3) (2005).

[2] F. Pattyn *et al.* "Benchmark experiments for higher-order and full-Stokes ice sheet models (ISMIP-HOM)". *Cryosphere* **2**(2) 95-108 (2008).

[3] M. Perego, M. Gunzburger, J. Burkardt. "Parallel finite-element implementation for higher-order ice-sheet models". *J. Glaciology* **58**(207) 76-88 (2012).

[4] J. Dukowicz, S.F. Price, W.H. Lipscomb. "Incorporating arbitrary basal topography in the variational formulation of ice-sheet models". *J. Glaciology* **57**(203) 461-466 (2011).

[5] A.G. Salinger, E. T. Phipps, R.A. Bartlett, G.A. Hansen, **I. Kalashnikova**, J.T. Ostien, W. Sun, Q. Chen, A. Mota, R.A. Muller, E. Nielsen, X. Gao. "Albany: A Component-Based Partial Differential Equation Code Build on Trilinos", submitted to *ACM. Trans. Math. Software*.

[6] M. Hoffman, **I. Kalashnikova**, M. Perego, S. Price, A. Salinger, R. Tuminaro. "A New Parallel, Scalable and Robust Finite Element Higher-Order Stokes Ice Sheet Dycore Built for Advanced Analysis", in preparation for submission to *The Cryosphere.*